



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:39 PM UTC

PDB ID : 1HRA / pdb_00001hra
Title : THE SOLUTION STRUCTURE OF THE HUMAN RETINOIC ACID
RECEPTOR-BETA DNA-BINDING DOMAIN
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Deposited on : 1993-07-25

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

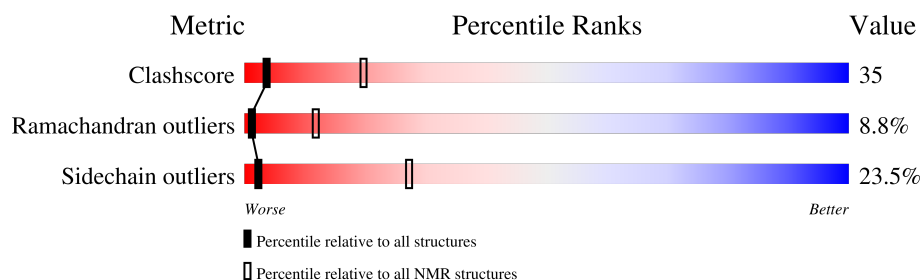
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	80	

2 Ensemble composition and analysis

This entry contains 15 models. Model 13 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:6-A:12, A:16-A:80 (72)	0.86	13

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 2, 6, 12, 13, 14
2	3, 7, 9
3	10, 15
Single-model clusters	4; 5; 8; 11

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 654 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RETINOIC ACID RECEPTOR.

Mol	Chain	Residues	Atoms					Trace
1	A	80	Total	C	N	O	S	0
			652	402	125	113	12	

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

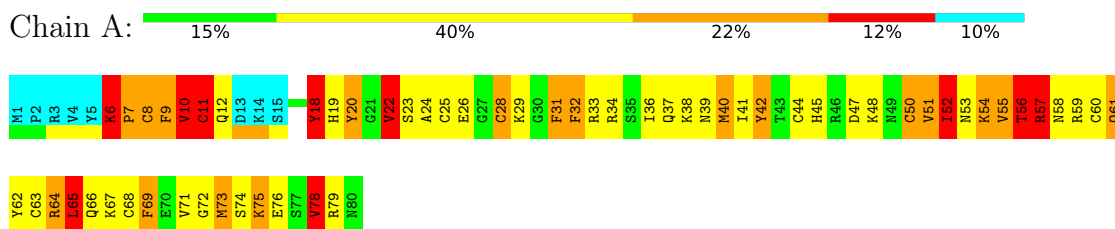
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: RETINOIC ACID RECEPTOR

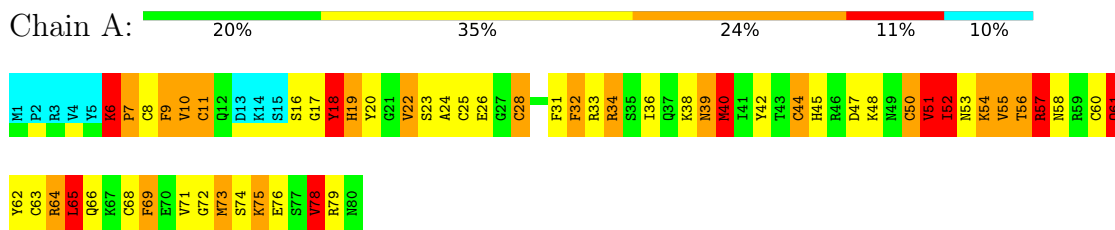


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

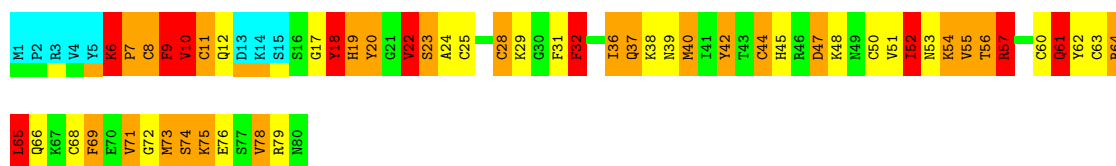
• Molecule 1: RETINOIC ACID RECEPTOR



4.2.2 Score per residue for model 2

• Molecule 1: RETINOIC ACID RECEPTOR

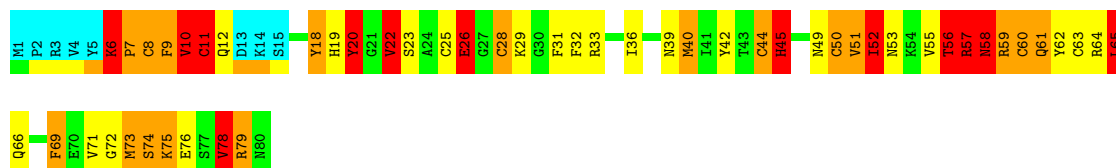




4.2.3 Score per residue for model 3

- Molecule 1: RETINOIC ACID RECEPTOR

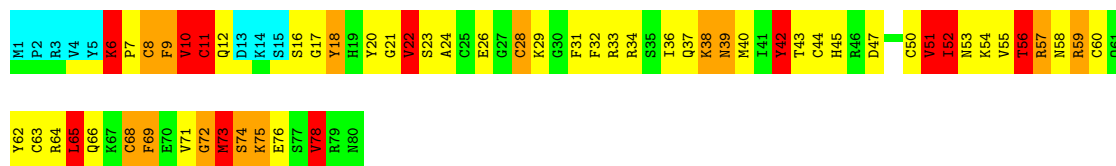
Chain A: 26% 26% 21% 16% 10%



4.2.4 Score per residue for model 4

- Molecule 1: RETINOIC ACID RECEPTOR

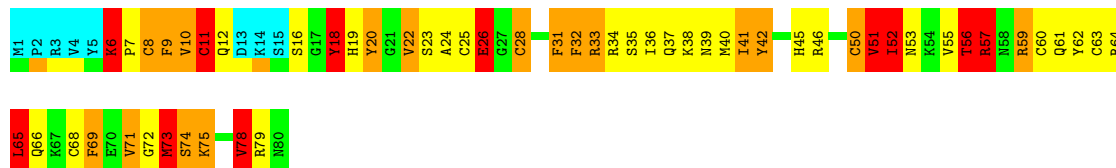
Chain A: 19% 41% 16% 14% 10%



4.2.5 Score per residue for model 5

- Molecule 1: RETINOIC ACID RECEPTOR

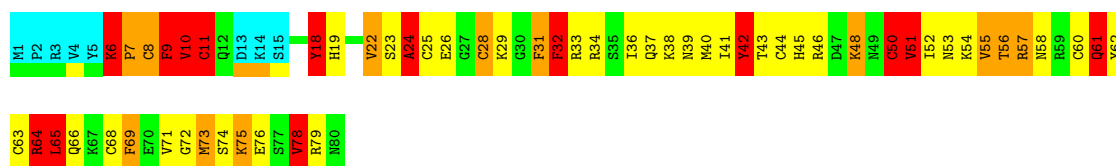
Chain A: 21% 34% 21% 14% 10%



4.2.6 Score per residue for model 6

- Molecule 1: RETINOIC ACID RECEPTOR

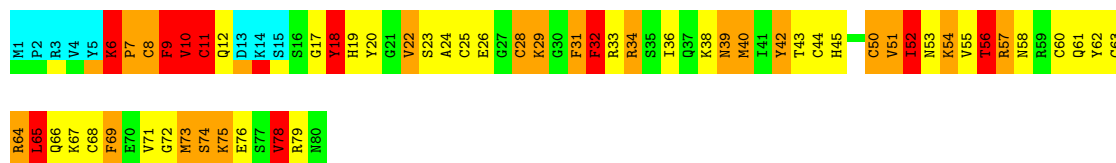
Chain A: 19% 39% 15% 18% 10%



4.2.7 Score per residue for model 7

- Molecule 1: RETINOIC ACID RECEPTOR

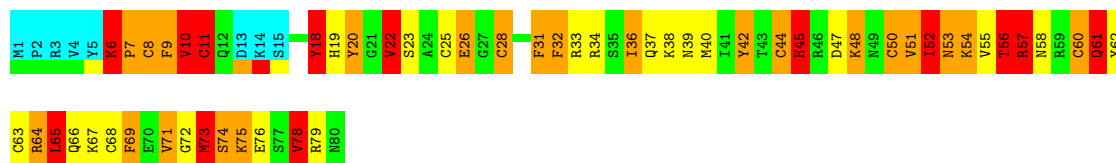
Chain A: 19% 35% 24% 12% 10%



4.2.8 Score per residue for model 8

- Molecule 1: RETINOIC ACID RECEPTOR

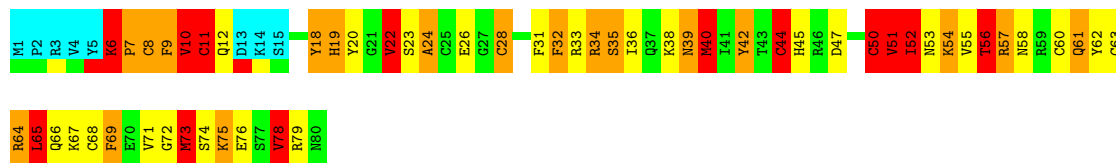
Chain A: 21% 25% 28% 16% 10%



4.2.9 Score per residue for model 9

- Molecule 1: RETINOIC ACID RECEPTOR

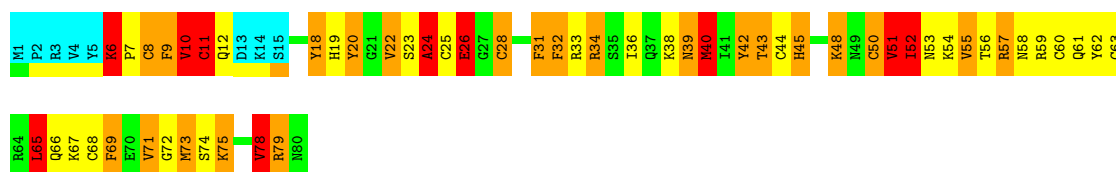
Chain A: 21% 30% 22% 16% 10%



4.2.10 Score per residue for model 10

- Molecule 1: RETINOIC ACID RECEPTOR

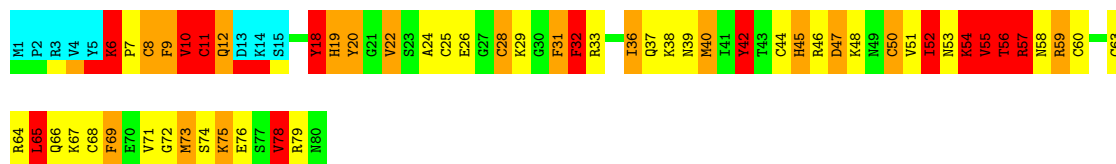
Chain A: 21% 29% 28% 12% 10%



4.2.11 Score per residue for model 11

- Molecule 1: RETINOIC ACID RECEPTOR

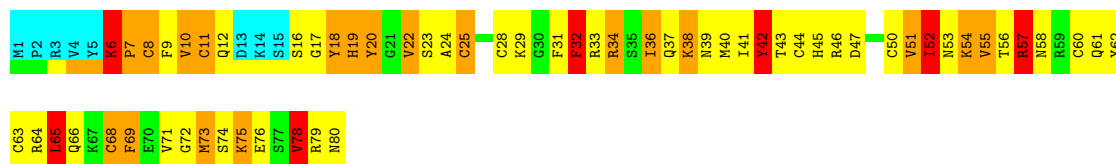
Chain A: 20% 32% 21% 16% 10%



4.2.12 Score per residue for model 12

- Molecule 1: RETINOIC ACID RECEPTOR

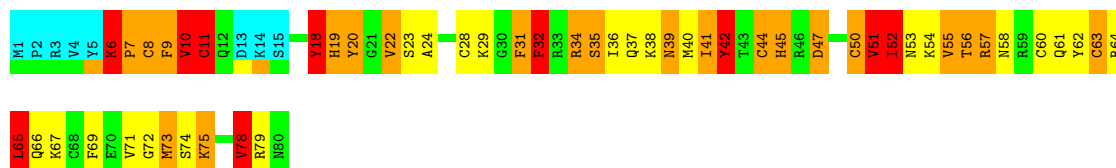
Chain A: 14% 44% 24% 9% 10%



4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: RETINOIC ACID RECEPTOR

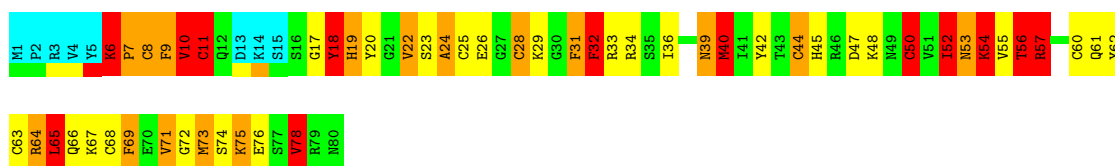
Chain A: 24% 28% 26% 12% 10%



4.2.14 Score per residue for model 14

- Molecule 1: RETINOIC ACID RECEPTOR

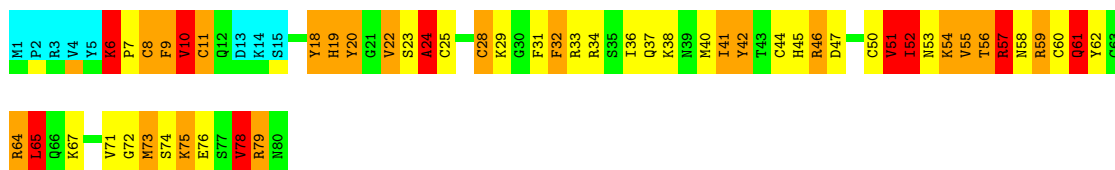
Chain A: 24% 30% 20% 16% 10%



4.2.15 Score per residue for model 15

- Molecule 1: RETINOIC ACID RECEPTOR

Chain A: 24% 30% 25% 11% 10%



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 15 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.06±0.02	1±1/594 (0.2± 0.1%)	2.21±0.05	28±4/788 (3.6± 0.5%)
All	All	1.06	14/8910 (0.2%)	2.21	421/11820 (3.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.1±0.2	21.6±3.7
All	All	1	324

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	76	GLU	CA-C	6.93	1.55	1.52	3	12
1	A	19	HIS	CA-C	6.47	1.55	1.52	6	1
1	A	19	HIS	CG-ND1	-5.36	1.32	1.38	15	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	56	THR	N-CA-CB	-12.50	99.96	111.59	2	10
1	A	11	CYS	CA-C-N	10.20	140.06	121.70	15	11
1	A	11	CYS	C-N-CA	10.20	140.06	121.70	15	11
1	A	8	CYS	N-CA-C	10.19	126.27	113.43	13	15
1	A	54	LYS	N-CA-C	10.14	122.61	110.44	11	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	56	THR	N-CA-C	9.94	124.01	109.69	3	9
1	A	18	TYR	N-CA-C	9.55	124.95	110.14	6	3
1	A	10	VAL	N-CA-CB	-9.36	99.07	111.90	13	14
1	A	55	VAL	N-CA-CB	-9.26	100.32	112.26	12	7
1	A	52	ILE	N-CA-CB	9.18	123.27	112.35	11	6
1	A	41	ILE	CA-C-N	8.88	137.69	121.70	5	2
1	A	41	ILE	C-N-CA	8.88	137.69	121.70	5	2
1	A	51	VAL	CA-C-N	8.81	137.56	121.70	6	1
1	A	51	VAL	C-N-CA	8.81	137.56	121.70	6	1
1	A	24	ALA	N-CA-C	8.69	123.56	109.40	9	4
1	A	10	VAL	N-CA-C	8.61	119.35	112.12	10	7
1	A	10	VAL	CA-CB-CG1	8.51	124.86	110.40	11	15
1	A	51	VAL	CB-CA-C	-8.10	99.83	110.84	1	9
1	A	39	ASN	N-CA-C	8.01	121.13	110.88	1	13
1	A	18	TYR	N-CA-CB	7.85	121.61	110.46	1	1
1	A	58	ASN	CA-C-N	7.83	135.79	121.70	8	2
1	A	58	ASN	C-N-CA	7.83	135.79	121.70	8	2
1	A	22	VAL	CA-CB-CG2	7.66	123.42	110.40	3	14
1	A	57	ARG	N-CA-C	7.22	118.06	107.88	11	1
1	A	6	LYS	CA-C-N	7.21	128.85	119.84	9	6
1	A	6	LYS	C-N-CA	7.21	128.85	119.84	9	6
1	A	74	SER	N-CA-C	7.10	119.19	109.11	8	4
1	A	52	ILE	CA-CB-CG1	7.02	122.33	110.40	15	9
1	A	43	THR	N-CA-C	7.01	125.74	110.80	6	1
1	A	28	CYS	N-CA-CB	6.93	120.42	110.16	4	12
1	A	57	ARG	CB-CA-C	6.92	124.19	110.42	12	8
1	A	28	CYS	N-CA-C	6.82	118.79	111.36	3	8
1	A	42	TYR	CB-CG-CD2	-6.80	110.60	120.80	13	5
1	A	22	VAL	CG1-CB-CG2	-6.78	95.89	110.80	7	15
1	A	56	THR	CA-C-N	6.63	134.21	121.54	5	7
1	A	56	THR	C-N-CA	6.63	134.21	121.54	5	7
1	A	57	ARG	N-CA-CB	-6.60	99.87	111.49	11	1
1	A	41	ILE	CB-CA-C	6.56	119.19	111.59	15	3
1	A	69	PHE	N-CA-C	6.49	119.18	111.71	7	13
1	A	73	MET	N-CA-C	-6.45	101.41	110.50	9	4
1	A	52	ILE	N-CA-C	6.45	118.34	107.18	13	2
1	A	6	LYS	N-CA-CB	-6.42	98.94	110.37	11	1
1	A	6	LYS	CA-C-O	-6.41	111.38	120.16	7	6
1	A	8	CYS	N-CA-CB	-6.40	100.66	110.20	15	3
1	A	11	CYS	O-C-N	-6.40	113.31	121.95	12	9
1	A	38	LYS	O-C-N	-6.34	113.81	122.81	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	12	GLN	N-CA-C	6.32	118.75	108.26	11	1
1	A	10	VAL	CB-CA-C	6.28	117.06	110.91	11	1
1	A	25	CYS	N-CA-CB	-6.25	101.41	110.47	11	7
1	A	12	GLN	N-CA-CB	-6.24	102.15	110.57	4	1
1	A	65	LEU	CB-CA-C	-6.16	101.20	110.88	13	2
1	A	19	HIS	CB-CG-CD2	-6.07	123.30	131.20	3	11
1	A	10	VAL	CA-CB-CG2	6.06	120.70	110.40	2	1
1	A	9	PHE	CA-CB-CG	5.98	119.78	113.80	2	3
1	A	50	CYS	CB-CA-C	5.97	122.30	110.42	14	3
1	A	18	TYR	CB-CG-CD2	-5.93	111.90	120.80	5	1
1	A	78	VAL	CA-CB-CG2	5.88	120.39	110.40	9	2
1	A	76	GLU	N-CA-CB	-5.87	101.18	111.04	1	3
1	A	11	CYS	N-CA-C	-5.85	100.91	109.63	11	1
1	A	45	HIS	N-CA-C	5.84	118.80	110.68	11	1
1	A	45	HIS	CA-CB-CG	5.83	119.63	113.80	3	1
1	A	51	VAL	O-C-N	-5.82	115.30	122.57	6	1
1	A	41	ILE	O-C-N	-5.76	115.36	122.57	13	2
1	A	78	VAL	CA-CB-CG1	5.73	120.15	110.40	12	11
1	A	25	CYS	N-CA-C	-5.71	100.68	109.76	12	1
1	A	44	CYS	CA-C-N	5.71	131.97	121.70	3	2
1	A	44	CYS	C-N-CA	5.71	131.97	121.70	3	2
1	A	78	VAL	N-CA-C	5.71	116.07	107.80	9	4
1	A	7	PRO	CA-C-N	5.70	130.33	120.58	12	2
1	A	7	PRO	C-N-CA	5.70	130.33	120.58	12	2
1	A	20	TYR	N-CA-C	5.66	117.92	108.02	10	5
1	A	31	PHE	CA-CB-CG	5.64	119.44	113.80	5	6
1	A	79	ARG	CA-CB-CG	-5.62	102.85	114.10	3	2
1	A	38	LYS	CA-C-N	5.57	131.73	121.70	2	1
1	A	38	LYS	C-N-CA	5.57	131.73	121.70	2	1
1	A	50	CYS	N-CA-C	5.55	118.33	107.57	7	1
1	A	11	CYS	CA-C-O	5.48	127.53	121.39	4	1
1	A	6	LYS	N-CA-C	5.45	121.86	109.81	13	6
1	A	41	ILE	N-CA-C	5.45	120.67	109.34	13	1
1	A	40	MET	N-CA-C	5.42	116.81	109.11	10	1
1	A	54	LYS	CA-C-N	5.37	130.69	122.69	12	1
1	A	54	LYS	C-N-CA	5.37	130.69	122.69	12	1
1	A	39	ASN	CA-CB-CG	5.30	117.90	112.60	7	2
1	A	57	ARG	CA-C-N	5.29	131.22	121.70	14	3
1	A	57	ARG	C-N-CA	5.29	131.22	121.70	14	3
1	A	36	ILE	N-CA-C	5.20	115.41	110.42	8	3
1	A	72	GLY	CA-C-N	5.19	128.08	120.71	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	72	GLY	C-N-CA	5.19	128.08	120.71	4	1
1	A	25	CYS	CA-C-N	5.16	131.40	121.54	8	3
1	A	25	CYS	C-N-CA	5.16	131.40	121.54	8	3
1	A	8	CYS	CA-C-N	5.14	130.95	121.70	11	1
1	A	8	CYS	C-N-CA	5.14	130.95	121.70	11	1
1	A	42	TYR	N-CA-C	5.13	118.98	111.34	10	1
1	A	22	VAL	CB-CA-C	5.11	119.67	111.29	9	1
1	A	50	CYS	N-CA-CB	-5.10	101.86	110.49	5	1
1	A	51	VAL	N-CA-C	5.10	119.94	109.34	5	1
1	A	36	ILE	CA-CB-CG2	5.09	119.16	110.50	2	1
1	A	6	LYS	CB-CA-C	5.08	120.19	110.17	7	1
1	A	67	LYS	N-CA-C	5.06	116.88	111.36	8	1
1	A	50	CYS	CA-CB-SG	5.06	126.03	114.40	9	1
1	A	49	ASN	CA-C-N	5.01	129.22	121.26	3	1
1	A	49	ASN	C-N-CA	5.01	129.22	121.26	3	1
1	A	59	ARG	CB-CA-C	5.01	119.38	111.72	11	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	18	TYR	CA	1

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	6	LYS	Peptide,Mainchain	15
1	A	9	PHE	Sidechain,Mainchain	15
1	A	18	TYR	Sidechain,Mainchain,Peptide	15
1	A	45	HIS	Peptide	15
1	A	55	VAL	Peptide,Mainchain	15
1	A	65	LEU	Mainchain	15
1	A	74	SER	Peptide	15
1	A	75	LYS	Peptide	15
1	A	32	PHE	Sidechain,Mainchain	13
1	A	62	TYR	Mainchain,Sidechain	13
1	A	50	CYS	Peptide,Mainchain	10
1	A	26	GLU	Mainchain	8
1	A	40	MET	Peptide,Mainchain	8
1	A	52	ILE	Peptide,Mainchain	8
1	A	7	PRO	Mainchain,Peptide	8

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	11	CYS	Mainchain,Peptide	8
1	A	42	TYR	Sidechain,Peptide	8
1	A	20	TYR	Sidechain,Mainchain	7
1	A	64	ARG	Peptide	7
1	A	71	VAL	Mainchain	7
1	A	56	THR	Mainchain,Peptide	6
1	A	24	ALA	Mainchain	6
1	A	34	ARG	Mainchain	5
1	A	47	ASP	Mainchain	4
1	A	22	VAL	Peptide,Mainchain	4
1	A	51	VAL	Mainchain,Peptide	4
1	A	54	LYS	Mainchain	3
1	A	57	ARG	Peptide,Mainchain	3
1	A	35	SER	Mainchain,Peptide	3
1	A	10	VAL	Mainchain	3
1	A	19	HIS	Sidechain	2
1	A	53	ASN	Peptide	2
1	A	31	PHE	Sidechain	2
1	A	23	SER	Mainchain	1
1	A	37	GLN	Mainchain,Peptide	1
1	A	58	ASN	Peptide	1
1	A	44	CYS	Peptide	1
1	A	59	ARG	Mainchain	1
1	A	63	CYS	Mainchain	1
1	A	41	ILE	Mainchain	1
1	A	46	ARG	Sidechain	1
1	A	79	ARG	Sidechain	1

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	584	0	573	41±5
All	All	8790	0	8585	610

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LYS:NZ	1:A:39:ASN:HD22	0.80	1.74	1	2
1:A:53:ASN:HD22	1:A:54:LYS:NZ	0.77	1.77	11	1
1:A:36:ILE:HA	1:A:40:MET:HG2	0.77	1.54	8	15
1:A:60:CYS:HB2	1:A:63:CYS:SG	0.77	2.19	5	1
1:A:37:GLN:HE21	1:A:38:LYS:NZ	0.76	1.77	12	7
1:A:38:LYS:HZ3	1:A:39:ASN:HD21	0.74	1.25	10	2
1:A:52:ILE:HG12	1:A:64:ARG:HG3	0.73	1.59	15	4
1:A:33:ARG:HB3	1:A:75:LYS:HE2	0.72	1.59	11	11
1:A:8:CYS:SG	1:A:11:CYS:HB3	0.72	2.24	14	7
1:A:38:LYS:HZ2	1:A:39:ASN:HD22	0.71	1.26	7	2
1:A:52:ILE:HG23	1:A:57:ARG:HB3	0.71	1.62	12	14
1:A:18:TYR:CZ	1:A:24:ALA:HB3	0.71	2.20	15	10
1:A:60:CYS:HB3	1:A:63:CYS:SG	0.71	2.26	13	9
1:A:31:PHE:CZ	1:A:65:LEU:HD22	0.69	2.22	9	15
1:A:33:ARG:HE	1:A:75:LYS:HZ3	0.69	1.27	7	4
1:A:52:ILE:H	1:A:67:LYS:NZ	0.69	1.85	10	1
1:A:78:VAL:HG22	1:A:79:ARG:HG3	0.69	1.65	3	5
1:A:22:VAL:HG21	1:A:73:MET:SD	0.68	2.28	8	14
1:A:6:LYS:HB2	1:A:7:PRO:HA	0.68	1.66	5	6
1:A:32:PHE:CE2	1:A:73:MET:HB2	0.66	2.25	13	15
1:A:75:LYS:HB3	1:A:78:VAL:HG11	0.66	1.68	11	15
1:A:37:GLN:HE21	1:A:38:LYS:HZ2	0.66	1.33	15	2
1:A:53:ASN:HD22	1:A:54:LYS:HZ3	0.66	1.34	11	1
1:A:56:THR:HG23	1:A:57:ARG:HG2	0.66	1.65	9	6
1:A:52:ILE:H	1:A:64:ARG:CZ	0.65	2.04	4	6
1:A:44:CYS:SG	1:A:63:CYS:HB3	0.65	2.30	14	6
1:A:51:VAL:H	1:A:52:ILE:HD13	0.65	1.51	7	3
1:A:8:CYS:HB3	1:A:10:VAL:H	0.65	1.52	6	8
1:A:22:VAL:HG11	1:A:73:MET:SD	0.64	2.33	10	12
1:A:52:ILE:HD12	1:A:57:ARG:O	0.63	1.93	11	1
1:A:68:CYS:HB3	1:A:73:MET:SD	0.63	2.33	11	10
1:A:54:LYS:HA	1:A:56:THR:HG22	0.63	1.71	2	1
1:A:52:ILE:HA	1:A:56:THR:OG1	0.63	1.94	14	7
1:A:51:VAL:C	1:A:52:ILE:HD13	0.62	2.18	12	9
1:A:38:LYS:NZ	1:A:39:ASN:HD21	0.62	1.91	10	2
1:A:44:CYS:HA	1:A:62:TYR:HB3	0.62	1.71	13	1
1:A:47:ASP:O	1:A:50:CYS:HB2	0.61	1.95	9	8
1:A:8:CYS:SG	1:A:25:CYS:HB2	0.61	2.36	2	2
1:A:33:ARG:NH1	1:A:37:GLN:HE22	0.60	1.94	6	1
1:A:8:CYS:HB3	1:A:11:CYS:H	0.60	1.55	9	7
1:A:6:LYS:NZ	1:A:6:LYS:H	0.60	1.93	5	1
1:A:22:VAL:HG22	1:A:23:SER:H	0.60	1.55	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ILE:HD13	1:A:75:LYS:O	0.60	1.96	13	5
1:A:11:CYS:HB2	1:A:52:ILE:HB	0.60	1.71	8	2
1:A:66:GLN:HA	1:A:69:PHE:HB2	0.59	1.74	13	14
1:A:51:VAL:N	1:A:52:ILE:HD13	0.59	2.12	7	3
1:A:33:ARG:HH21	1:A:75:LYS:HZ2	0.59	1.40	12	2
1:A:57:ARG:HB2	1:A:59:ARG:HB3	0.58	1.74	5	3
1:A:33:ARG:HE	1:A:75:LYS:NZ	0.58	1.96	7	3
1:A:34:ARG:HH22	1:A:61:GLN:NE2	0.58	1.95	10	2
1:A:6:LYS:HB2	1:A:8:CYS:H	0.57	1.59	7	9
1:A:53:ASN:H	1:A:56:THR:HG21	0.57	1.58	15	4
1:A:52:ILE:HG23	1:A:57:ARG:H	0.56	1.59	11	1
1:A:44:CYS:H	1:A:48:LYS:NZ	0.56	1.99	6	1
1:A:9:PHE:CD2	1:A:71:VAL:HG21	0.56	2.36	4	11
1:A:18:TYR:CZ	1:A:23:SER:HA	0.55	2.36	3	4
1:A:22:VAL:HG22	1:A:23:SER:O	0.55	2.02	14	10
1:A:28:CYS:O	1:A:32:PHE:HB2	0.55	2.01	8	15
1:A:52:ILE:H	1:A:67:LYS:HZ2	0.55	1.44	10	1
1:A:75:LYS:HA	1:A:78:VAL:HG21	0.54	1.80	7	15
1:A:50:CYS:SG	1:A:60:CYS:HB3	0.54	2.43	8	3
1:A:18:TYR:OH	1:A:24:ALA:HB3	0.54	2.03	11	7
1:A:54:LYS:NZ	1:A:57:ARG:HH12	0.53	1.99	9	1
1:A:33:ARG:HH21	1:A:75:LYS:NZ	0.53	2.01	8	2
1:A:64:ARG:HD3	1:A:67:LYS:HB2	0.53	1.81	15	3
1:A:54:LYS:H	1:A:54:LYS:NZ	0.53	2.02	14	1
1:A:9:PHE:CD1	1:A:71:VAL:HG21	0.53	2.39	7	2
1:A:54:LYS:H	1:A:54:LYS:HZ2	0.53	1.44	14	1
1:A:57:ARG:HA	1:A:58:ASN:C	0.52	2.29	7	9
1:A:50:CYS:SG	1:A:58:ASN:HB3	0.52	2.44	3	1
1:A:33:ARG:NE	1:A:75:LYS:HZ3	0.52	2.00	7	1
1:A:46:ARG:HG3	1:A:60:CYS:HB2	0.52	1.82	15	3
1:A:20:TYR:OH	1:A:29:LYS:HG2	0.52	2.05	12	4
1:A:6:LYS:O	1:A:8:CYS:HB2	0.52	2.05	2	1
1:A:32:PHE:CZ	1:A:73:MET:HG3	0.51	2.41	4	13
1:A:51:VAL:H	1:A:58:ASN:ND2	0.51	2.03	11	1
1:A:35:SER:O	1:A:40:MET:HB3	0.51	2.05	13	1
1:A:37:GLN:HE21	1:A:38:LYS:HZ3	0.51	1.48	4	1
1:A:37:GLN:HB3	1:A:38:LYS:HZ2	0.50	1.64	8	1
1:A:36:ILE:CG2	1:A:78:VAL:HG12	0.50	2.37	2	5
1:A:75:LYS:HZ1	1:A:79:ARG:CZ	0.50	2.19	8	2
1:A:37:GLN:NE2	1:A:79:ARG:HE	0.50	2.04	6	1
1:A:78:VAL:HG22	1:A:79:ARG:HG2	0.50	1.82	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LYS:HZ2	1:A:79:ARG:HH21	0.50	1.48	11	1
1:A:75:LYS:HE3	1:A:78:VAL:HG11	0.50	1.83	11	4
1:A:9:PHE:HB2	1:A:23:SER:H	0.50	1.66	9	1
1:A:63:CYS:SG	1:A:64:ARG:N	0.50	2.85	5	7
1:A:8:CYS:H	1:A:9:PHE:HA	0.50	1.67	8	6
1:A:22:VAL:HG22	1:A:23:SER:N	0.50	2.22	9	4
1:A:75:LYS:HE3	1:A:78:VAL:CG1	0.49	2.37	6	3
1:A:8:CYS:N	1:A:9:PHE:HA	0.49	2.22	5	5
1:A:8:CYS:HB3	1:A:10:VAL:N	0.49	2.23	15	6
1:A:53:ASN:HD22	1:A:54:LYS:N	0.49	2.04	8	2
1:A:33:ARG:CZ	1:A:37:GLN:HE22	0.49	2.20	6	1
1:A:8:CYS:CB	1:A:11:CYS:H	0.49	2.21	7	3
1:A:38:LYS:NZ	1:A:39:ASN:ND2	0.49	2.60	10	2
1:A:29:LYS:HZ2	1:A:33:ARG:CZ	0.48	2.21	12	2
1:A:12:GLN:HG2	1:A:53:ASN:O	0.48	2.08	3	1
1:A:41:ILE:H	1:A:42:TYR:HB3	0.48	1.69	13	1
1:A:55:VAL:HB	1:A:56:THR:HG23	0.48	1.84	11	2
1:A:37:GLN:HE21	1:A:38:LYS:HZ1	0.48	1.46	12	1
1:A:60:CYS:SG	1:A:61:GLN:N	0.47	2.87	15	6
1:A:34:ARG:NE	1:A:39:ASN:HD21	0.47	2.06	13	1
1:A:6:LYS:HB3	1:A:9:PHE:O	0.47	2.09	1	2
1:A:32:PHE:CD2	1:A:75:LYS:HB2	0.47	2.45	4	11
1:A:51:VAL:O	1:A:57:ARG:HA	0.47	2.09	8	1
1:A:64:ARG:HG3	1:A:67:LYS:HB3	0.47	1.87	14	1
1:A:65:LEU:HB3	1:A:66:GLN:NE2	0.47	2.25	11	4
1:A:37:GLN:HE21	1:A:75:LYS:NZ	0.47	2.07	6	1
1:A:18:TYR:CE2	1:A:23:SER:HA	0.47	2.45	8	1
1:A:36:ILE:HD11	1:A:65:LEU:HD12	0.46	1.87	9	10
1:A:50:CYS:HB3	1:A:63:CYS:HB3	0.46	1.87	10	1
1:A:6:LYS:HB2	1:A:7:PRO:CA	0.46	2.38	5	1
1:A:51:VAL:HG12	1:A:53:ASN:ND2	0.46	2.26	5	2
1:A:6:LYS:C	1:A:8:CYS:H	0.46	2.19	12	2
1:A:53:ASN:ND2	1:A:54:LYS:H	0.46	2.09	11	1
1:A:20:TYR:OH	1:A:75:LYS:HG2	0.46	2.10	13	2
1:A:37:GLN:NE2	1:A:38:LYS:NZ	0.45	2.64	13	2
1:A:36:ILE:HG22	1:A:78:VAL:HG12	0.45	1.86	2	3
1:A:48:LYS:NZ	1:A:48:LYS:H	0.45	2.08	10	1
1:A:34:ARG:HG2	1:A:39:ASN:HD21	0.45	1.70	7	2
1:A:52:ILE:HD12	1:A:57:ARG:HB3	0.45	1.88	5	2
1:A:42:TYR:HD2	1:A:61:GLN:HB2	0.45	1.72	6	1
1:A:38:LYS:HZ3	1:A:39:ASN:HD22	0.44	1.50	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:TYR:HB2	1:A:74:SER:H	0.44	1.71	3	1
1:A:51:VAL:O	1:A:56:THR:HB	0.44	2.12	1	2
1:A:54:LYS:HZ1	1:A:57:ARG:HH12	0.44	1.55	9	1
1:A:12:GLN:HB2	1:A:52:ILE:O	0.44	2.13	2	2
1:A:18:TYR:HD2	1:A:20:TYR:O	0.44	1.94	8	1
1:A:64:ARG:O	1:A:68:CYS:HB2	0.44	2.13	4	2
1:A:52:ILE:HD13	1:A:52:ILE:N	0.44	2.28	14	2
1:A:59:ARG:CZ	1:A:59:ARG:H	0.43	2.26	4	2
1:A:46:ARG:HG3	1:A:60:CYS:SG	0.43	2.54	5	1
1:A:52:ILE:HG22	1:A:53:ASN:O	0.43	2.14	1	2
1:A:24:ALA:C	1:A:26:GLU:H	0.43	2.22	5	1
1:A:36:ILE:HG22	1:A:78:VAL:O	0.43	2.13	1	1
1:A:12:GLN:HG2	1:A:53:ASN:C	0.43	2.38	3	1
1:A:78:VAL:HA	1:A:79:ARG:HA	0.43	1.48	13	4
1:A:7:PRO:O	1:A:24:ALA:C	0.43	2.62	7	4
1:A:40:MET:HE2	1:A:42:TYR:CE1	0.43	2.49	5	2
1:A:57:ARG:HG3	1:A:59:ARG:HH21	0.43	1.74	3	1
1:A:53:ASN:CG	1:A:54:LYS:H	0.43	2.22	7	1
1:A:46:ARG:HG2	1:A:60:CYS:HB2	0.42	1.91	11	1
1:A:44:CYS:SG	1:A:47:ASP:C	0.42	3.03	14	1
1:A:44:CYS:N	1:A:48:LYS:NZ	0.42	2.68	6	1
1:A:35:SER:HB3	1:A:40:MET:HB3	0.42	1.92	9	1
1:A:53:ASN:CG	1:A:54:LYS:N	0.42	2.77	7	1
1:A:40:MET:HB2	1:A:42:TYR:CZ	0.42	2.50	4	1
1:A:17:GLY:HA3	1:A:18:TYR:HA	0.42	1.70	12	4
1:A:8:CYS:HA	1:A:24:ALA:HA	0.42	1.92	7	1
1:A:40:MET:HE2	1:A:42:TYR:CZ	0.41	2.50	11	1
1:A:51:VAL:H	1:A:58:ASN:HB3	0.41	1.75	4	3
1:A:63:CYS:C	1:A:64:ARG:HE	0.41	2.23	7	1
1:A:10:VAL:HG11	1:A:67:LYS:HB3	0.41	1.93	10	1
1:A:25:CYS:HB3	1:A:28:CYS:H	0.41	1.74	1	1
1:A:10:VAL:HG13	1:A:64:ARG:HE	0.41	1.75	4	1
1:A:40:MET:HE2	1:A:42:TYR:OH	0.41	2.15	9	1
1:A:59:ARG:H	1:A:59:ARG:NE	0.41	2.13	4	1
1:A:56:THR:HB	1:A:57:ARG:H	0.41	1.60	15	1
1:A:50:CYS:O	1:A:64:ARG:HD3	0.41	2.16	12	1
1:A:10:VAL:HG12	1:A:68:CYS:SG	0.41	2.55	2	1
1:A:10:VAL:HG21	1:A:67:LYS:C	0.41	2.41	11	1
1:A:46:ARG:HB2	1:A:50:CYS:SG	0.41	2.56	11	1
1:A:48:LYS:H	1:A:48:LYS:NZ	0.41	2.14	8	1
1:A:34:ARG:HG2	1:A:38:LYS:HZ1	0.41	1.76	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:TYR:HD1	1:A:73:MET:HB3	0.40	1.76	3	1
1:A:50:CYS:HB3	1:A:63:CYS:CB	0.40	2.46	10	1
1:A:26:GLU:O	1:A:29:LYS:HG3	0.40	2.16	3	1
1:A:8:CYS:SG	1:A:28:CYS:SG	0.40	3.19	4	1
1:A:9:PHE:HD2	1:A:71:VAL:HG21	0.40	1.74	9	1
1:A:43:THR:HA	1:A:44:CYS:HA	0.40	1.75	10	1
1:A:73:MET:H	1:A:73:MET:HG2	0.40	1.48	4	1
1:A:44:CYS:HA	1:A:45:HIS:C	0.40	2.41	8	1
1:A:35:SER:O	1:A:36:ILE:HG13	0.40	2.15	13	1
1:A:31:PHE:HZ	1:A:65:LEU:HD22	0.40	1.72	10	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	71/80 (89%)	44±2 (62±3%)	20±2 (29±3%)	6±2 (9±2%)	1	12
All	All	1065/1200 (89%)	665 (62%)	306 (29%)	94 (9%)	1	12

All 18 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	72	GLY	15
1	A	6	LYS	11
1	A	57	ARG	10
1	A	19	HIS	9
1	A	61	GLN	9
1	A	44	CYS	6
1	A	26	GLU	6
1	A	22	VAL	5
1	A	52	ILE	5
1	A	16	SER	4
1	A	43	THR	3
1	A	50	CYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	17	GLY	2
1	A	20	TYR	2
1	A	58	ASN	1
1	A	21	GLY	1
1	A	51	VAL	1
1	A	42	TYR	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	66/74 (89%)	50±2 (76±3%)	16±2 (24±3%)	2	27
All	All	990/1110 (89%)	757 (76%)	233 (24%)	2	27

All 40 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	6	LYS	15
1	A	10	VAL	15
1	A	11	CYS	15
1	A	42	TYR	15
1	A	65	LEU	15
1	A	73	MET	15
1	A	78	VAL	15
1	A	52	ILE	14
1	A	61	GLN	9
1	A	48	LYS	7
1	A	18	TYR	7
1	A	32	PHE	7
1	A	34	ARG	7
1	A	29	LYS	6
1	A	56	THR	6
1	A	51	VAL	5
1	A	57	ARG	4
1	A	20	TYR	4
1	A	45	HIS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	59	ARG	4
1	A	44	CYS	4
1	A	53	ASN	4
1	A	54	LYS	4
1	A	40	MET	3
1	A	39	ASN	3
1	A	60	CYS	3
1	A	38	LYS	3
1	A	12	GLN	3
1	A	50	CYS	3
1	A	68	CYS	2
1	A	64	ARG	2
1	A	26	GLU	2
1	A	37	GLN	1
1	A	58	ASN	1
1	A	33	ARG	1
1	A	41	ILE	1
1	A	43	THR	1
1	A	74	SER	1
1	A	79	ARG	1
1	A	80	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided